Convergence of Mimetic Finite Difference Method for Diffusion Problems on Polyhedral Meshes

Franco Brezzi

University of Pavia, Italy
brezzi@imati.cnr.it

Konstantin Lipnikov **Mikhail Shashkov**

Los Alamos National Laboratory, USA
lipnikov@lanl.gov, shashkov@lanl.gov

Acknowledgments

- FIRB 2001 and PRIN 2003 projects of Italian MIUR.
- DOE/ASCR program in Applied Mathematical Sciences.
- Advance Simulation and Computing (ASC) program.

Contents

- Motivation
- Mimetic finite difference method
- Theoretical assumptions
- Main results
- Possible extensions
- Conclusion

Motivation

- Sources of polyhedral meshes:
  - meshing of complex geometries
  - adaptive mesh refinement methods
  - multi-block meshes (non-matching, hybrid)
  - mesh reconnection methods
  - moving mesh methods

Motivation

- "*... The tests carried out so far indicate that our polyhedral meshes lead to superior convergence rates and accuracy relative to tetrahedral meshes and comparable to those of high-quality hexahedral meshes (where both can be generated).*"

  [CD adapco Group]

Mimetic finite difference method

$$\vec{F} = -K\,\mathrm{grad}\,p, \quad \mathrm{div}\vec{F} = b, \qquad \mathrm{div} = -(K\,\mathrm{grad})^*, \quad \mathrm{Null}(\mathrm{grad}) = const$$

$$MFD$$

$$\boldsymbol{F}^h = -\mathcal{G}\,\boldsymbol{p}^h, \quad \mathcal{DIV}\boldsymbol{F}^h = \boldsymbol{b}^h, \qquad \mathcal{DIV} = -\mathcal{G}^*, \quad \mathrm{Null}(\mathcal{G}) = const$$

Mimetic finite difference method

$$\boxed{\vec{F} = -K\,\mathrm{grad}\,p, \quad \mathrm{div}\vec{F} = b, \qquad \mathrm{div} = -(K\,\mathrm{grad})^*, \quad \mathrm{Null}(\mathrm{grad}) = const}$$

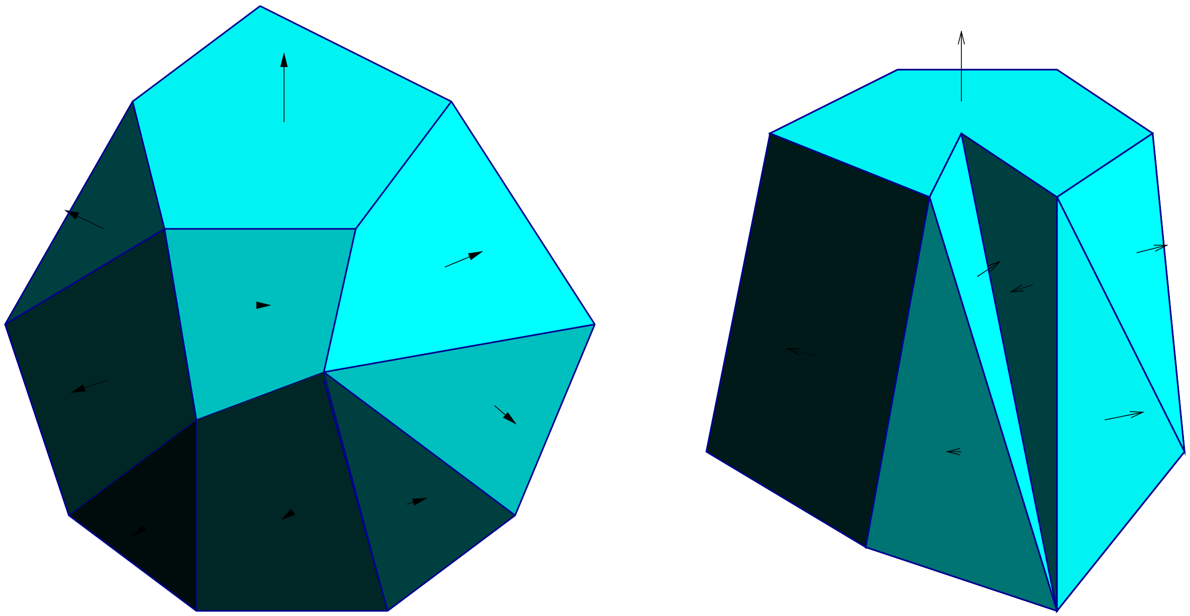
Four-step methodology:

1. Define degrees of freedom for $\boldsymbol{p}^h \in Q_h$ and $\boldsymbol{F}^h \in X_h$
2. Discretize the mass balance equation, $\mathcal{DIV}\colon X_h \to Q_h$
3. Equip discrete spaces with scalar products $[\cdot\,,\,\cdot]_Q$ and $[\cdot\,,\,\cdot]_X$
4. Derive the discrete flux operator, $\mathcal{G}\colon Q_h \to X_h$, from Green's formula

$$\boxed{\boldsymbol{F}^h = -\mathcal{G}\,\boldsymbol{p}^h, \quad \mathcal{DIV}\boldsymbol{F}^h = \boldsymbol{b}^h, \qquad \mathcal{DIV} = -\mathcal{G}^*, \quad \mathrm{Null}(\mathcal{G}) = const}$$

Mimetic finite difference method

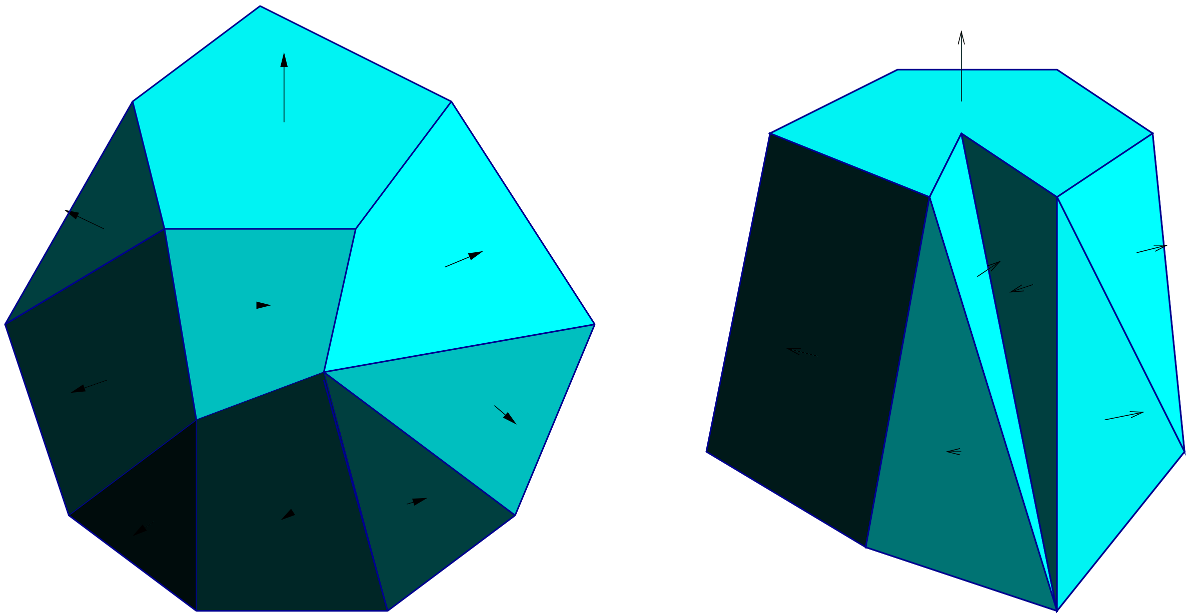
Step 1. Define degrees of freedom for $\boldsymbol{p}^h \in Q_h$ and $\boldsymbol{F}^h \in X_h$



- $\boldsymbol{p}^h$ is constant on each polyhedron, $\dim(Q_h) = \#elements$
  - $(\boldsymbol{p}^h)_E$ is the degree of freedom associated with element E
  - define the interpolated function $\boldsymbol{p}^I \in Q_h$ as follows: $(\boldsymbol{p}^I)_E = \dfrac{1}{|E|}\displaystyle\int_E p(x)\,\mathrm{d}x$

Mimetic finite difference method

Step 1. Define degrees of freedom for $p^h \in Q_h$ and $\boldsymbol{F}^h \in X_h$



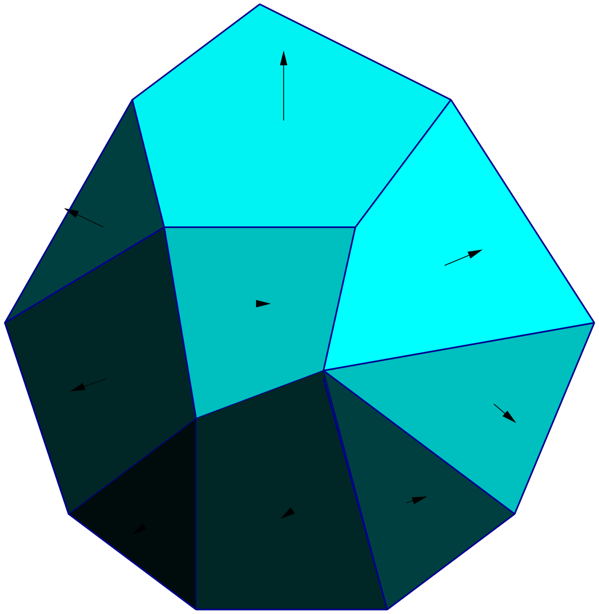
- $\boldsymbol{F}^h$ is constant on each face, $\quad \dim(X_h) = \# faces$
  - $(\boldsymbol{F}^h)_f$ is the normal velocity component associated with face f
  - define the interpolated function $\boldsymbol{F}^I \in X_h$ as follows: $(\boldsymbol{F}^I)_f = \dfrac{1}{|f|}\displaystyle\int_f \vec{F}\cdot\vec{n}\,\mathrm{d}x$

Mimetic finite difference method

Steps 2. Discretize the mass balance equation, $\mathcal{DIV}\colon X_h \to Q_h$

Gauss' theorem:

$$\operatorname{div}\vec{F} = \lim_{|E|\to 0} \frac{1}{|E|} \oint_{\partial E} \vec{F}\cdot\vec{n}\, dx$$



The definition of $\boldsymbol{F}^h$ gives

$$\left(\mathcal{DIV}\,\boldsymbol{F}^h\right)_E = \frac{1}{|E|} \sum_{f\in\partial E} (\boldsymbol{F}^h)_f\, |f|$$

Mimetic finite difference method

Step 3. Equip discrete spaces with scalar products $[\cdot\,,\,\cdot]_Q$ and $[\cdot\,,\,\cdot]_X$

- $$[\boldsymbol{p}^h,\,\boldsymbol{q}^h]_Q = \sum_{E\in\Omega_h} (\boldsymbol{p}^h)_E\,(\boldsymbol{q}^h)_E|E|$$

- $$[\boldsymbol{F}^h,\,\boldsymbol{G}^h]_X = \sum_{E\in\Omega_h} [\boldsymbol{F}^h,\,\boldsymbol{G}^h]_E$$

  where

  $$[\boldsymbol{F}^h,\,\boldsymbol{G}^h]_E = \sum_{i,j=1}^{k_E} M_{E,i,j}\,(\boldsymbol{F}^h)_{f_i}\,(\boldsymbol{G}^h)_{f_j}$$

  and M_E is an SPD matrix.

Mimetic finite difference method

Steps 4. Derive the discrete flux operator, $\mathcal{G}: Q_h \to X_h$, from Green's formula

- The continuous operators div and $(K\,\mathrm{grad})$ satisfy

$$\int_\Omega \vec{F} \cdot K^{-1}(K\,\mathrm{grad} p)\,\mathrm{d}x = -\int_\Omega p\,\mathrm{div}\vec{F}\,\mathrm{d}x.$$

- We enforce that the discrete operators $\mathcal{DIV}$ and $\mathcal{G}$ satisfy

$$[\boldsymbol{F}^h, \mathcal{G}\,\boldsymbol{p}^h]_X = -[\boldsymbol{p}^h, \mathcal{DIV}\,\boldsymbol{F}^h]_Q \qquad \forall \boldsymbol{p}^h \in Q_h \quad \forall \boldsymbol{F}^h \in X_h.$$

Mimetic finite difference method

$$\vec{F} = -K\,\mathrm{grad}\,p, \quad \mathrm{div}\vec{F} = b, \qquad \mathrm{div} = -(K\,\mathrm{grad})^*, \quad \mathrm{Null(grad)} = const$$

Four-step methodology:

1. Define degrees of freedom for $\boldsymbol{p}^h \in Q_h$ and $\boldsymbol{F}^h \in X_h$
2. Discretize the mass balance equation, $\mathcal{DIV}\colon X_h \to Q_h$
3. Equip discrete spaces with scalar products $[\cdot\,,\,\cdot]_Q$ and $[\cdot\,,\,\cdot]_X$
4. Derive the discrete flux operator, $\mathcal{G}\colon Q_h \to X_h$, from Green's formula

$$\boldsymbol{F}^h = -\mathcal{G}\,\boldsymbol{p}^h, \quad \mathcal{DIV}\boldsymbol{F}^h = \boldsymbol{b}^h, \qquad \mathcal{DIV} = -\mathcal{G}^*, \quad \mathrm{Null}(\mathcal{G}) = const$$

Problem assumptions

- Regularity and ellipticity of K.

  Every component of K is in $W^1_\infty(\Omega)$ and K is strongly elliptic:

$$\kappa_* \|\mathbf{v}\|^2 \leq \mathbf{v}^T K(\mathbf{x})\, \mathbf{v} \leq \kappa^* \|\mathbf{v}\|^2$$

  for all $\mathbf{v} \in \Re^3$ and $\mathbf{x} \in \Omega$.

- Assumptions on the domain Ω.

  Ω is a polyhedron with a Lipschitz continuous boundary.

Mesh assumptions

- Number of faces and edges.

  Every element E has at most N_f faces, and each face f has at most N_e edges.

- Volumes, areas, and lengths.

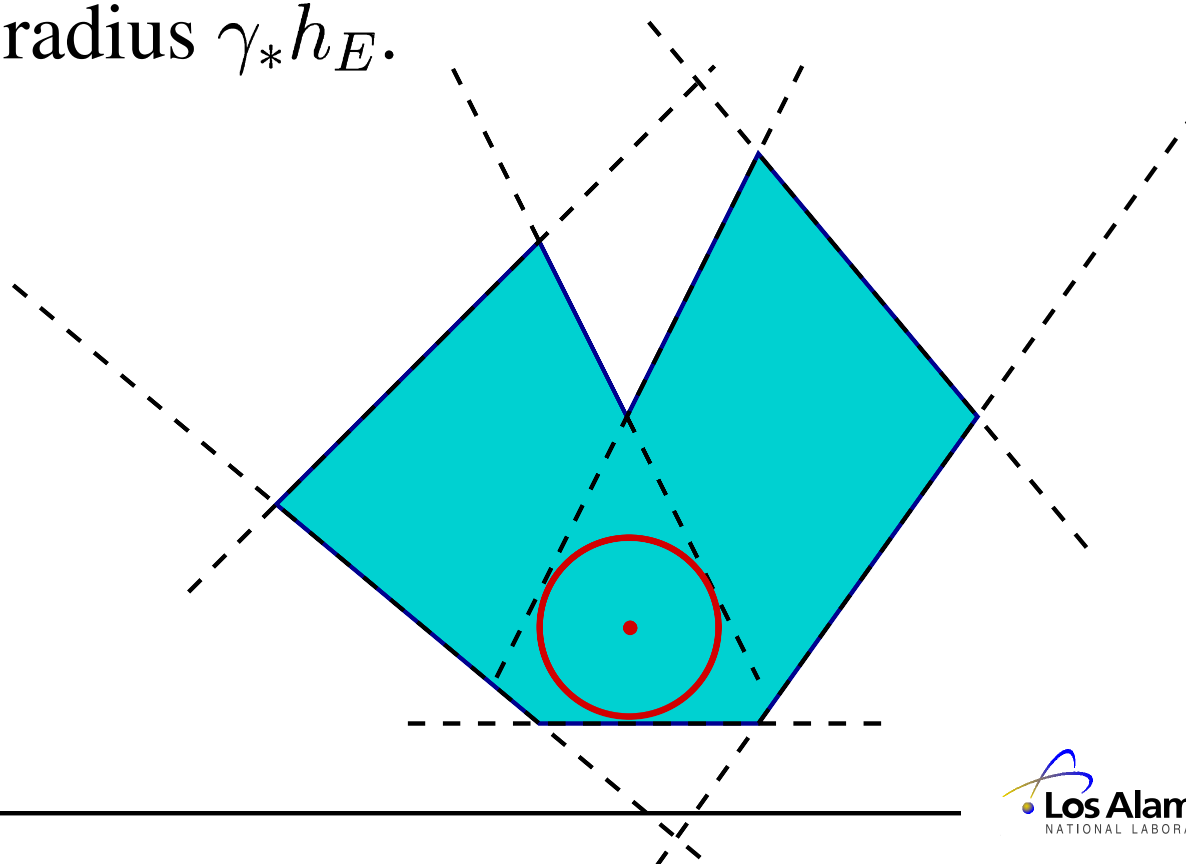
  $\exists$ three positive constants v_*, a_* and ℓ_* such that

$$v_* h_E^3 \leq |E|, \quad a_* h_E^2 \leq |f|, \quad \ell_* h_E \leq |e|$$

  where h_E is the diameter of E.

Mesh assumptions

- Star-shaped faces.
  - Mesh faces are flat.
  - $\exists$ a positive constant γ_* s.t. each face f of element E is star-shaped w.r.t. every point of the disk D_f of radius $\gamma_* h_E$.

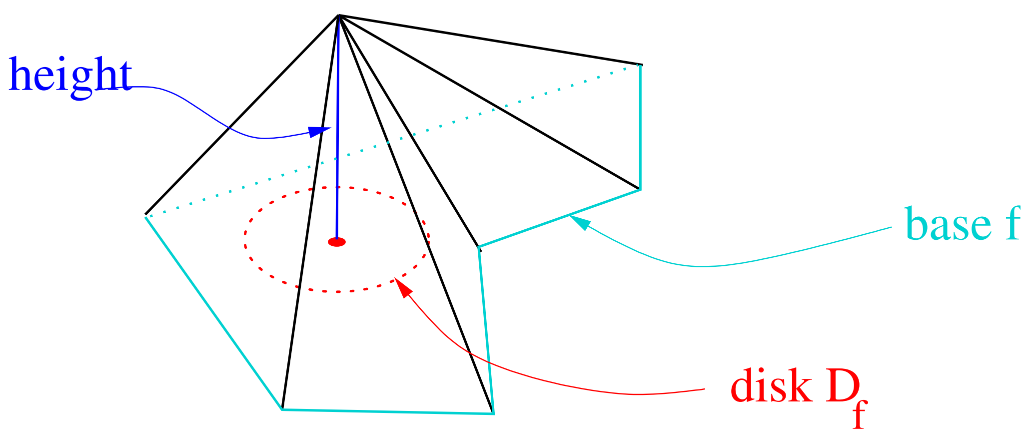


Mesh assumptions

- The pyramid property.

For every face f of element E, $\exists$ a pyramid P_E^f s.t.

- P_E^f is contained in E
- its base is equal to f
- its height is equal to $\gamma_* \, h_E$
- its vertex is projected to the center of disk D_f



Mesh assumptions

- Star-shaped elements.

  $\exists$ a positive number τ_* s.t. every element E is star-shaped w.r.t. every point of a sphere of radius $\tau_* \, h_E$.

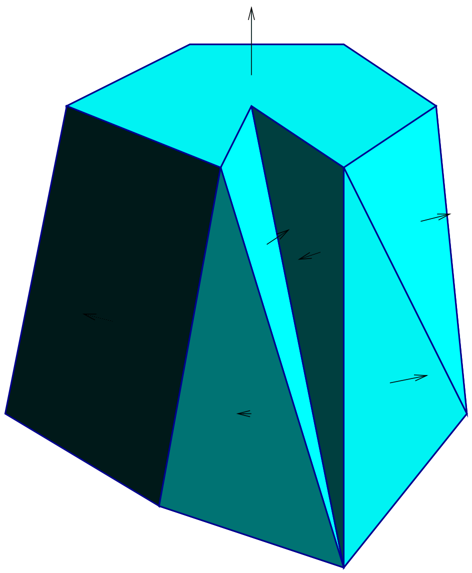
Mesh assumptions

The assumptions forbid:

- anisotropic (stretched) elements
- stretched faces
- small 2D angles

The assumptions allow:

- regular meshes
- degenerate elements
- non-convex elements



Scalar product assumptions

- Stability of $[\cdot,\,\cdot]_E$.

  $\exists$ two positive constants s_* and S^* s.t., for every $\boldsymbol{G}^h \in X_h$ and for every element E, one has

$$s_*\,|E| \sum_{f\in\partial E} (\boldsymbol{G}^h)_f^2 \leq \,[\boldsymbol{G}^h,\,\boldsymbol{G}^h]_E \,\leq S^*\,|E| \sum_{f\in\partial E} (\boldsymbol{G}^h)_f^2.$$

Scalar product assumptions

- Stability of $[\cdot,\ \cdot]_E$.

  $\exists$ two positive constants s_* and S^* s.t., for every $\boldsymbol{G}^h \in X_h$ and for every element E, one has

$$s_* \, |E| \sum_{f \in \partial E} (\boldsymbol{G}^h)_f^2 \leq \, [\boldsymbol{G}^h,\, \boldsymbol{G}^h]_E \, \leq S^* \, |E| \sum_{f \in \partial E} (\boldsymbol{G}^h)_f^2 .$$

  - convergence proofs based on relationships with MFE methods and Strang's first lemma can NOT be used.

Scalar product assumptions

- Consistency of $[\cdot,\ \cdot]_E$.

  For every element E, every linear function q^1 and every $\boldsymbol{G}^h \in X_h$, we have

$$[(K\,\nabla q^1)^I,\ \boldsymbol{G}^h]_E = \int\limits_{\partial E} q^1\,\boldsymbol{G}^h\,\mathrm{d}x - \int\limits_{E} q^1\,(\mathcal{DIV}\,\boldsymbol{G}^h)_E\,\mathrm{d}x$$

Scalar product assumptions

- Consistency of $[\cdot,\ \cdot]_E$.

  For every element E, every linear function q^1 and every $\boldsymbol{G}^h \in X_h$, we have

$$[(K\,\nabla q^1)^I,\, \boldsymbol{G}^h]_E = \int_{\partial E} q^1\, \boldsymbol{G}^h\, \mathrm{d}x - \int_{E} q^1\, (\mathcal{DIV}\, \boldsymbol{G}^h)_E\, \mathrm{d}x$$

  - for divergence-free functions, we get

$$[(K\,\nabla q^1)^I,\, \boldsymbol{G}^h]_E = \int_{\partial E} q^1\, \boldsymbol{G}^h\, \mathrm{d}x.$$

Scalar product assumptions

- Consistency of $[\cdot,\,\cdot]_E$.

For every element E, every linear function q^1 and every $\boldsymbol{G}^h \in X_h$, we have

$$[(K\,\nabla q^1)^I,\, \boldsymbol{G}^h]_E = \int_{\partial E} q^1\, \boldsymbol{G}^h\, \mathrm{d}x - \int_E q^1\, (\mathcal{DIV}\, \boldsymbol{G}^h)_E\, \mathrm{d}x$$

- for $q^1 = 1$, we get the definition of $\mathcal{DIV}$:

$$\left(\mathcal{DIV}\, \boldsymbol{G}^h\right)_E = \frac{1}{|E|} \sum_{f \in \partial E} (\boldsymbol{G}^h)_f\, |f|$$

Scalar product assumptions

- Consistency of $[\cdot,\,\cdot]_E$.

  For every element E, every linear function q^1 and every $\boldsymbol{G}^h \in X_h$, we have

$$[(K\,\nabla q^1)^I,\,\boldsymbol{G}^h]_E = \int\limits_{\partial E} q^1\,\boldsymbol{G}^h\,\mathrm{d}x - \int\limits_{E} q^1\,(\mathcal{DIV}\,\boldsymbol{G}^h)_E\,\mathrm{d}x$$

  - we are left with 3 possible choice for q^1:

$$q^1 = x, \qquad q^1 = y, \qquad q^1 = z.$$

  - we get a linear system for the coefficients of M_E (NO lifting operator)

Main results

- stability analysis
- estimate for the vector variable
- 1st estimate for the scalar variable
- link to methods using lifting operators
- 2nd estimate for the scalar variable

Main results

- Stability analysis.

  Define mesh norms:

$$|||\boldsymbol{p}^h|||_Q^2 := [\boldsymbol{p}^h,\, \boldsymbol{p}^h]_Q, \qquad |||\boldsymbol{F}^h|||_X^2 := [\boldsymbol{F}^h,\, \boldsymbol{F}^h]_X$$

and

$$|||\boldsymbol{F}^h|||_{div}^2 := |||\boldsymbol{F}^h|||_X^2 + \sum_{E \in \Omega_h} h_E^2 \, \|\mathcal{DIV}\,\boldsymbol{F}^h\|_{L_2(E)}^2.$$

Main results

- Stability analysis (cont.)

For every $\boldsymbol{q}^h \in Q_h$, there exists $\boldsymbol{G}^h \in X_h$ s.t.

$$[\mathcal{DIV}\, \boldsymbol{G}^h,\, \boldsymbol{q}^h]_Q \geq \beta_* \, |||\boldsymbol{G}^h|||_{div} \, |||\boldsymbol{q}^h|||_Q$$

where β_* is a constant independent of $\boldsymbol{q}^h$, $\boldsymbol{G}^h$ and Ω_h.

Main results

- Estimate for the vector variables.

Theorem. Let $(p,\ \vec{F})$ be the continuous solution, $(\boldsymbol{p}^h,\ \boldsymbol{F}^h)$ be the discrete solution and $\boldsymbol{F}^I$ be the interpolant of $\vec{F}$. Then

$$|||\boldsymbol{F}^I - \boldsymbol{F}^h|||_X \leq\ C^*\, h\, \|p\|_{H^2(\Omega)},$$

where

$$h = \max_{E \in \Omega_h} h_E.$$

Main results

- 1st estimate for the scalar variables.

Theorem. Let $(p,\ \vec{F})$ be the continuous solution, $(\boldsymbol{p}^h,\ \boldsymbol{F}^h)$ be the discrete solution and $\boldsymbol{p}^I$ be the interpolant of p. For *convex* domain Ω, we get

$$|||\boldsymbol{p}^I - \boldsymbol{p}^h|||_Q \leq C^*\, h\, \left(||p||_{H^2(\Omega)} + ||b||_{H^1(\Omega)}\right)$$

where b is the source term.

Main results

- Link to methods using lifting operators.

Consider a lifting operator R_E with the properties:

- preserves normal components: $R_E(\boldsymbol{G}^h) \cdot \vec{n} = (\boldsymbol{G}^h)_f \quad \forall f \in \partial E$
- preserves constant divergence: $\operatorname{div}\left(R_E(\boldsymbol{G}^h)\right) = \left(\mathcal{DIV}\, \boldsymbol{G}^h\right)_E$
- exact for constant vectors $\vec{G}_0$: $R_E(\boldsymbol{G}_0^I) = \vec{G}_0$

Then

$$[\boldsymbol{F}^h, \boldsymbol{G}^h]_E := \int_E K^{-1} R_E(\boldsymbol{F}^h) \cdot R_E(\boldsymbol{G}^h)\, \mathrm{d}x$$

satisfies the scalar product assumptions.

Main results

- 2nd estimate for the scalar variables.

Theorem Let $(p,\ \vec{F})$ be the continuous solution, $(\boldsymbol{p}^h,\ \boldsymbol{F}^h)$ be the discrete solution and $\boldsymbol{p}^I$ be the interpolant of p. Let Ω be *convex* domain and the lifting operator R_E satisfy

$$\| R_E(\boldsymbol{G}^I) - \vec{G}\|_{L_2(E)} \leq \ C^*_{Ra}\, h_E\, \|\vec{G}\|_{(H^1(E))^3}$$

for all $\vec{G}$. Then

$$|||\boldsymbol{p}^I - \boldsymbol{p}^h|||_Q \leq \ C^*\, h^2\ \left(\|p\|_{H^2(\Omega)} + \|b\|_{H^1(\Omega)}\right).$$

Numerical methods for computing M_E

For every linear function q^1 and every $\boldsymbol{G}^h \in X_h$, we have

$$[(K\,\nabla q^1)^I,\, \boldsymbol{G}^h]_E = \int_{\partial E} q^1\, \boldsymbol{G}^h\, \mathrm{d}x - \int_E q^1\, (\mathcal{DIV}\, \boldsymbol{G}^h)_E\, \mathrm{d}x.$$

It results in 3 sets of equations with unknown matrix M_E:

$$M_E\, \boldsymbol{a}_i = \boldsymbol{c}_i, \qquad i = 1, 2, 3,$$

where

$$\boldsymbol{a}_1 = (K\,\nabla x)^I, \quad \boldsymbol{a}_2 = (K\,\nabla y)^I, \quad \boldsymbol{a}_3 = (K\,\nabla z)^I.$$

Numerical methods for computing M_E

- matrix M_E has $k(k+1)/2$ unknown entries:

$$\begin{pmatrix} m_{11} & m_{12} & m_{13} & m_{14} \\ m_{12} & m_{22} & m_{23} & m_{24} \\ m_{13} & m_{23} & m_{33} & m_{34} \\ m_{14} & m_{24} & m_{34} & m_{44} \end{pmatrix} \qquad \text{for} \quad k=4 \quad (tetrahedron)$$

- 3 equations, $M_E\,\boldsymbol{a}_i = \boldsymbol{c}_i$, give a linear system

$$A\,m = C$$

  - it has at most $3k-3$ linear independent equations
  - it is always compatible
  - the solution vector m is not unique

Numerical methods for computing M_E

- We search for a solution maximizing 2-norm of diagonal elements:

$$\color{red}{m} = \arg\max_{m} \sum_{i=1}^{k} m_{ii}^2$$

and minimizing 2-norm of off-diagonal elements.

- The it trick is to modify the original equations:

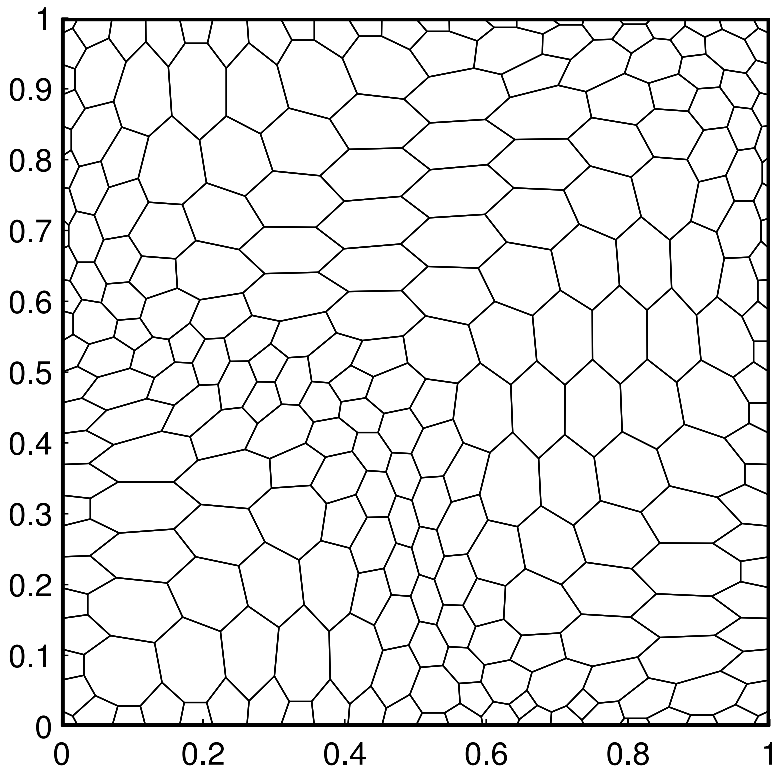
$$N_E\, \boldsymbol{a}_i = (\alpha_E I - \color{blue}{M_E})\boldsymbol{a}_i = \alpha_E \boldsymbol{a}_i - \boldsymbol{c}_i$$

and to use the LAPACK routine giving a minimal norm solution.

Numerical methods for computing M_E

Let $p(x,\, y) = x^3\, y^2 + x\, \cos(xy)\, \sin(x)$, $\alpha_E = 5|E|$ and

$$K(x,\, y) = \begin{pmatrix} (x+1)^2 + y^2 & -xy \\ -xy & (x+1)^2 \end{pmatrix}.$$



l	$\|\|\|p^I - p^h\|\|\|_Q$	$\|\|\|F^I - F^h\|\|\|_X$
1	7.79e-1	2.00e-0
2	1.38e-1	9.73e-1
3	2.96e-2	4.01e-1
4	7.00e-3	1.46e-1
5	1.72e-3	5.32e-2
rate	2.19	1.32

Extensions of the methodology

- Straightforward extensions:
  - h^2-curved faces (almost flat faces)
  - problems with a lack of elliptic regularity
- Possible extensions:
  - other PDEs (Maxwell, linear elasticity)
  - essentially curved faces

Conclusion

- We developed a new methodology for the design and the analysis of the MFD method.
- We proved stability of the discretization.
- We proved optimal convergence estimates.
- We analyzed numerically a new algorithm for computing M_E.